Chanalyzer: New Release

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Abstract

Here is the description of the improvements and updates in the new Chanalyzer release.

The changes can be roughly classified into three main contributions:

1. the introduction of a new step (Step E) aimed at providing new metrics for the retrieved channel and new visual representations of it;

2. a modified pipeline (including new steps and programs) to deal with occluded channels;

3. a modified pipeline (including new steps and programs) if a pathway is provided as input.

1 New Step: E - Metrics and Visualization

We have integrated in Chanalyzer some metrics for evaluating, analyzing, and visually representing the channel retrieved by the previous steps (A - D2). The tools and the code have been introduced in this repository https://github.com/rea1991/GEO-Nav-methods and discussed in this article [RFB23].

Specifically, Step E takes as input the centerline endowed with radius values of the maximal inscribed balls returned by Step D2 and it provides as output of Step E:

- metrics about the centerline of the identified channel, such as:
    - the number of vertices,
    - the length,
    - the straightness;
- informative visualizations of the channel:
    - the centerline of the retrieved channel colored in accordance with the radius values adopting the coolwarm colormap of Matplotlib (represented as a point cloud and encoded into an OFF file),
    - the retrieved channel (as a collection of spheres) colored in accordance with the radius values adopting the coolwarm colormap of Matplotlib (represented as a point cloud and encoded into an OFF file),
    - a PNG file representing the graph of the radius functions of the centerline of the considered model.

2 Modified Pipeline in case of Occluded Channels

We propose here a modified/improved pipeline for dealing with molecular structures which present a channel that is occluded and does not completely pass through the molecular surface from side to side.

3 Modified Pipeline in case of Input Pathway

We have experienced that for certain molecular structures, the portion of surface returned by Chanalyzer includes the correct channel but it also contains large portions of the molecular surface which do not have such property. A possible way to improve the result in such a situation consists in including information about the pathway and exploiting it to correctly identify the portion of the Chanalyzer output being a channel. Obviously this pipeline is compatible with the above proposed one aimed at dealing with occluded channels.

4 Minor updates

We have:

- corrected some typos and modified the NanoShaper Installation Guide;

- added a python program to convert structures expressed in a 'pqr' format into a 'xyzr' format.

References

[RFB23] Andrea Raffo, Ulderico Fugacci, and Silvia Biasotti. Geo-nav: A geometric dataset of voltage-gated sodium channels. *Computers & Graphics*, 115:285–295, 2023.